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INTERSTELLAR DETECTION OF CCC AND HIGH-PRECISION LABORATORY MEASUREMENTS NEAR 2 THz

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ABSTRACT

We describe more fully our original tentative interstellar detection of the triatomic pure carbon chain molecule, CCC, in absorption toward the Galactic center source Sgr B2. C_3 was detected with the Kuiper Airborne Observatory (KAO) by observing the $R(2)$ bending vibration-rotation transition $(0, 1^1, 0) \leftarrow (0, 0^0, 0)$ near 65.7 cm^{-1} during one of the last flights of KAO. The $R(2)$ absorption line detected toward Sgr B2 is centered at 63.7(5) km s^{-1}, with $\Delta V(\mathrm{FWHM}) = 8.3(9)$ km s^{-1} and a peak absorption of 18(3)%. This original tentative interstellar detection of C_3 has recently been confirmed by J. Cernicharo et al. through observation of a total of nine absorption lines, including the same $R(2)$ line with the *Infrared Space Observatory*. We also present highly precise new laboratory measurements of 10 rovibrational transition frequencies of the ν_2 bending mode of C_3, which have been obtained with the Cologne Sideband Spectrometer for Terahertz Application.

Subject headings: ISM: individual (Sagittarius B2) — ISM: molecules — line: identification — methods: laboratory — techniques: spectroscopic

On-line material: color figure

1. INTRODUCTION

Ever since the discovery of the carbon chain molecules, HC_nN, with $n = 1, 3, 5, \ldots$, in dense interstellar clouds by T. Oka, H. W. Kroto, and coworkers in 1976 (Avery et al. 1976), there has been much interest in such species because of possible roles in dust grain dynamics (Mathis 1993; Dorschner & Henning 1995), interstellar chemistry (Guelin et al. 1997; Herbst & Leung 1989), laboratory spectroscopy (Thaddeus & McCarthy 1999), the diffuse interstellar bands (Douglas 1977), and the unidentified infrared emission bands (Gillett, Forrest, & Merrill 1973). The interstellar molecular architecture is dominated by carbon-bearing molecules, among which the carbon chains with various terminal groups (see, e.g., Thaddeus & McCarthy 1999; Winnewisser, Herbst, & Ungerechts 1992) are particularly conspicuous because of their high interstellar molecular abundance.

Carbon chain molecules appear in two different forms: those that carry a permanent electric dipole moment and those that are nonpolar. Polar species can be measured by their rotational spectra. Unsaturated polyynes, e.g., HC_nN with $n = 1, 3, 5, \ldots, 11$, with alternating single and triple carbon-carbon bonds and cumulenes, e.g., linear carbon chain radicals, C_nH with $n = 2, 4, \ldots, 8$, displaying successive carbon double bonds, represent the dominant structural theme of the molecules so far identified in space (see, e.g., Thaddeus et al. 1998). Pure carbon chain molecules, however, are nonpolar. They exhibit no pure rotational spectrum, are considerably more difficult to observe, and thus much less is known about them. They can, however, be detected through their infrared active transitions. Many carbon chain molecules display infrared active, low-energy bending vibrations. All pure carbon chain molecules, except C_2, are expected to exhibit bending vibrations in the range 30–150 cm^{-1}, i.e., in the far-infrared region, or what might also be called the terahertz domain, depending on the technique used.

Triatomic carbon, C_3, exhibits one bending vibration (ν_2) at 63.42 cm^{-1} or 1.901 THz in addition to its mid-infrared spectrum of the ν_3 antisymmetric stretching mode (Matsumura et al. 1988; Kawaguchi et al. 1989). While C_3 and C_5 have been observed via their antisymmetric stretching mode spectra (ν_3 of C_3 near 2040 cm^{-1} and ν_3 of C_5 near 2164 cm^{-1}) in the circumstellar shell of the late-type star IRC +10216 (Hinkle, Keady, & Bernath 1988; Bernath, Hinkle, & Keady 1989), this approach is not applicable to cold clouds without IR background sources.

In 1990, the Berkeley group suggested the possibility of detecting pure carbon chain molecules in dense and cold interstellar clouds via far-infrared bending rovibrational transitions (Van Orden et al. 1995). One of the prime targets was the interstellar detection of C_3, laboratory terahertz spectra that had been measured for the first time by the Berkeley group (Schmuttenmaer et al. 1990) and recently refined and extended in the Cologne laboratories. The feasibility of this approach was demonstrated with the first observation of the $R(2)$ bending rovibrational transition of C_3 in Sgr B2 by using the Betz/Boreiko heterodyne receiver aboard the Kuiper Airborne Observatory (KAO; Betz & Boreiko 1993; Boreiko & Betz 1996; Van Orden et al. 1995). Unfortunately, this first and at that time tentative detection could not be confirmed by additional observations, e.g., of an independent second transition, because of the termination of KAO operations. However, by these combined laboratory and interstellar measurements on C_3, a firm route has been established to the general study of pure carbon chains (and indeed, many other nonpolar molecules) in the dense and cold interstellar environment via their rovibrational bending transitions. With the advent of new airplane-borne telescopes by the year 2002 with SOFIA, one of the main tasks in unraveling the riddles associated with the abundance, architecture, and excitation mechanisms of interstellar carbon seems to rest in the availability of the appropriate rest frequencies of the bending rovibrational transitions of the different carbon chain molecules.

In this Letter we describe our 1994 detection of C_3, elucidate the conditions prevailing in the region of Sgr B2 producing the absorption signals, and present the most recent laboratory measurements of the ν_2 band at 63.42 cm^{-1} or 1.901 THz of C_3.

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2. OBSERVATIONS AND RESULTS

The first laboratory measurements of the C_3 bending rotation transitions made by Schmuttenmaer et al. (1990) with tunable far-IR laser spectroscopy of a laser vaporized carbon plasma were used to design a search for this species in the interstellar medium, using the Betz/Boreiko receiver on board the KAO. An initial search for the $Q(4)$ transition at 1896.707 GHz was conducted toward two Galactic star-forming regions, the IRc2 source in Orion A and W3 during a KAO flight from NASA Ames Research Center on 1994 January 28. The $R(2)$ transition at 1968.595 GHz was searched toward the Galactic center source Sgr B2 during the 1994 KAO Southern Skies Expedition 5 in New Zealand. No emission lines arising from these transitions were detected in any of the three observed sources. However, a weak absorption signal, displayed in Figure 1, was observed toward Sgr B2. This new interstellar absorption feature we identified as the $R(2)$ transition of C_3. Unfortunately, as a result of the grounding of the KAO, no confirmation of this initial detection could be obtained by us. Very recently, confirmation came by the identification of the $R(2)$ and eight other bending rotation transitions in the far-IR data from the *Infrared Space Observatory* (*ISO*; Cernicharo, Goicoechea, & Caux 2000).

The transition dipole moment of the ν_2 bending mode of C_3 has been calculated to be 0.4371 D (Jensen, Rolling, & Almföf 1992). From this we obtain a value for the Einstein A-coefficient of about 7×10^{-3} s^{-1} for the dipole transitions in the ν_2 rovibrational band. The critical density required to thermalize the $\nu_2 = 1$ level is estimated to 3×10^8 cm^{-3}, assuming the temperature of the H_2 gas to be about 50–100 K and provided that the excitation is thermal. Such densities are observed only near the cores of dense molecular clouds. Therefore, emission signals arising from the deexcitation of the ν_2 mode of C_3 should be detectable in only high-density regions. Populating by IR photons provides another important mechanism for pumping the ν_2 levels of C_3. For the excitation of ν_2 of C_3 to be dominated by IR photons, the continuum emission by the surrounding interstellar dust has to be strong, as is the case for Sgr B2. From the Betz/Boreiko receiver sensitivity, we have estimated that the minimum total column density required to detect these emissions is 3×10^{14} cm^{-2} for a 100 K gas.

These constraints are relaxed somewhat when a source of continuum radiation at far-IR wavelengths is present, permitting molecular absorption lines to be observed. Figure 1 displays the Sgr B2 spectrum that we observed at the wavelength of the $R(2)$ line of the C_3 bending mode. From a fit to the experimental KAO data, the following parameters have been derived from the $R(2)$ absorption line:

line position $V_{\rm LSR} = 63.7(5)$ km s^{-1},

line width (FWHM) $\Delta V = 8.3(9)$ km s^{-1},

peak absorption = 18(3)%.

The LSR velocity of 63.7 ± 0.5 km s^{-1} of the peak absorption of C_3 is characteristic of absorption lines of other molecules such as the rotation-inversion transitions of NH_3, which were the first molecular lines detected in absorption toward Sgr B2 (Winnewisser, Churchwell, & Walmsley 1979). In fact, the Sgr B2 molecular cloud breaks into essentially two hot ($T_{\rm kin} \sim 200$ K) and dense [$n(H_2) > 10^6$ cm^{-3}] cores, Sgr B2(N) and Sgr B2(M), which display submillimeter line emission and continuum dust emission. Located in front of them is a cooler but more extended low-density envelope from which lines of many molecules, such as NH_3, NH_2, HCN, CN, and many others have been detected with velocities of $V_{\rm LSR} \sim 66$ km s^{-1} toward Sgr B2(M) and at 63 and 81 km s^{-1} against Sgr B2(N) (see, e.g., Martín-Pintado et al. 1990).

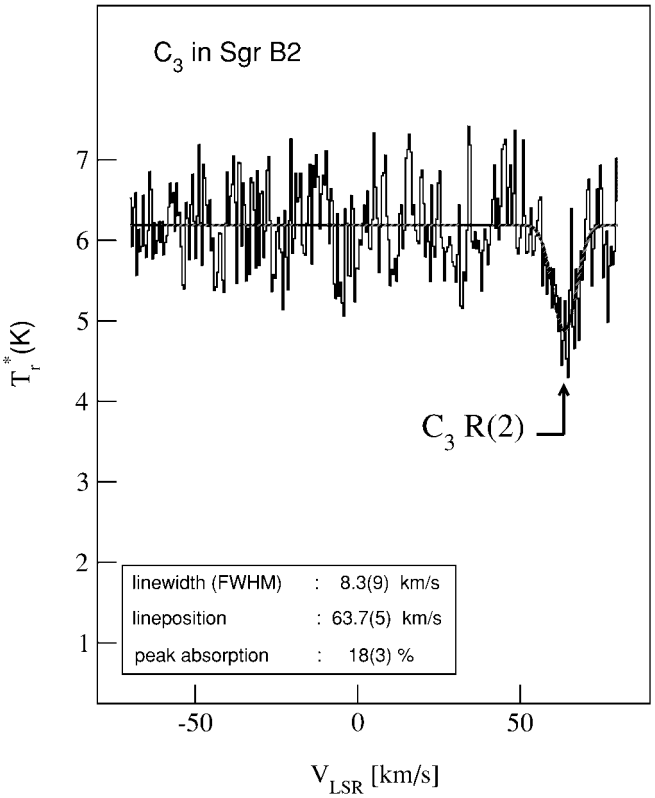

FIG. 1.—C_3 absorption line toward Sgr B2 using KAO. The peak occurring at 63.7(5) km s^{-1} has been assigned as the $R(2)$ transition of the ν_2 bending mode of C_3 at 1968.5954(1) GHz. The solid curve shows the fit of a Voigt profile to the data, yielding a line width (FWHM) of 8.3(9) km s^{-1} with a negligible Lorentzian width and a peak absorption of 18(3)%. [*See the electronic edition of the Journal for a color version of this figure.*]

With an angular separation of somewhat less than 50″, observed spectra with insufficient angular resolution cannot be used to discern between the velocity structure associated with the two sources. On the other hand, the widths of these absorption lines are all rather similar, around 15 km s^{-1}. For NH_2 the precise values for the LSR velocity is $V_{\rm LSR} = 66 \pm 2$ km s^{-1} and the associated velocity dispersion $\Delta V = 13.8 \pm 1.2$ km s^{-1} (van Dishoeck et al. 1993). LSR velocities and line widths of other molecules observed toward the same position of Sgr B2, e.g., H_2CO (Martín-Pintado et al. 1990), are consistent with the aforementioned parameters.

The $R(2)$ line of C_3 observed with KAO is surprisingly narrow [8.3(9) km s^{-1}], nearly half of the average value of 15 km s^{-1} obtained for the line widths of a wide sample of other molecules, indicating that the C_3 absorption occurs at the hydrodynamically most quiet part of the absorbing cloud, i.e., probably in a fairly narrow region of the extended envelope, which might also be the coolest part. In contrast to this result, the $R(2)$ line observed by *ISO* toward Sgr B2 is very broad, covering almost 200 km s^{-1}, perhaps indicating that it stems from the warm molecular gas close to the Galactic center and/or from foreground cold material intersecting the line of sight. As also noted by Cernicharo et al. (2000), a more trivial explanation would be remaining

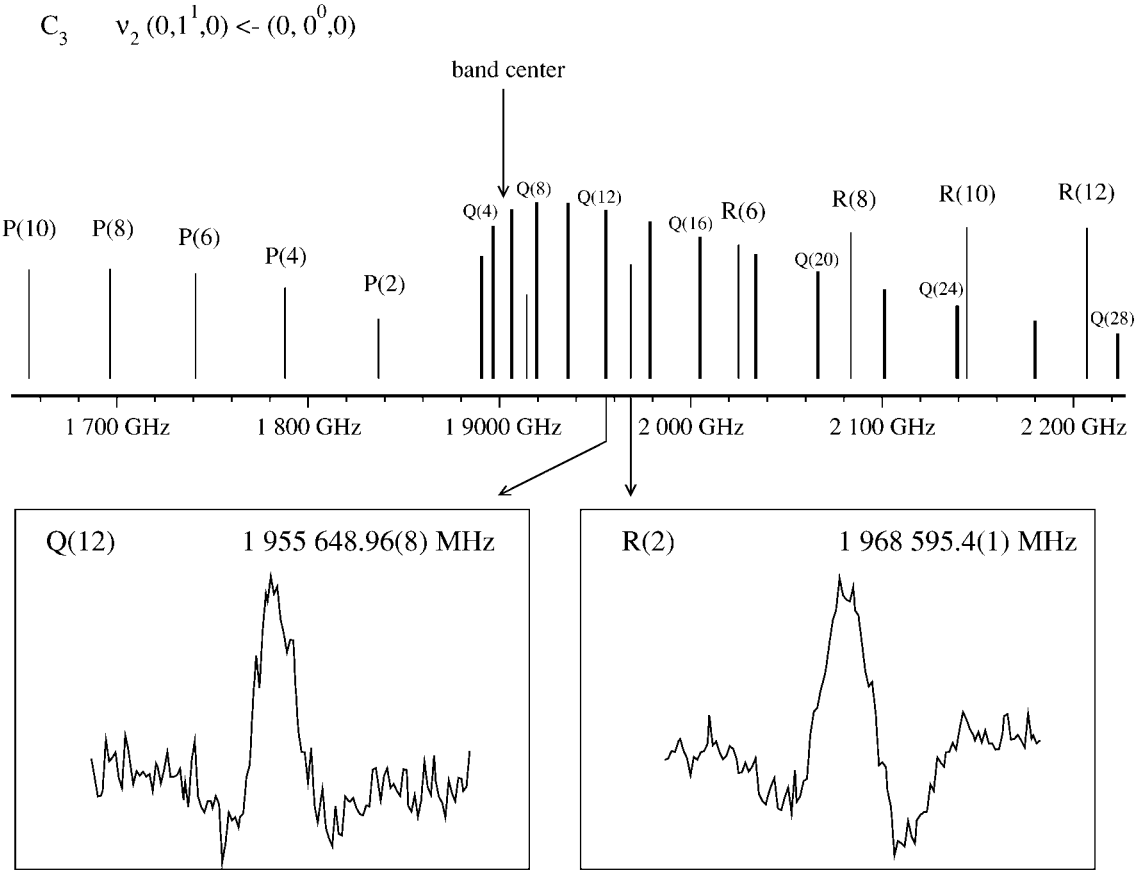

FIG. 2.—Calculated stick spectrum of the C_3 bending fundamental mode ν_2 with two selected laboratory recordings of the $Q(12)$ and $R(2)$ transitions. The band origin is centered at 63.416523(4) cm^{-1} or 1901.179(1) GHz. The rotational constant B differs by 3% between ground and excited states, causing a widely spread Q-branch.

instrumental/baseline effects due to insufficient velocity coverage. However, the $R(4)$ and $R(6)$ lines observed with *ISO* show also broad absorption to the blue in addition to the absorption feature produced by Sgr B2. This 50 km s^{-1} absorption feature is common to all *ISO* data, i.e., in addition to the three R lines, also $P(4)$ and $Q(4)$, $Q(6)$, $Q(8)$, $Q(10)$, and $Q(12)$, indicating that all *ISO* data are spectrally underresolved by the limited resolving power of 9500 (Cernicharo 2000).

TABLE 1

MEASURED FAR-IR ROVIBRATIONAL TRANSITIONS OF C_3, THE n_2 BENDING MODE $(0, 1^1, 0) \leftarrow (0, 0^0, 0)$

Transition	ν_{Cologne}[a] (MHz)	ν_{Berkeley}[b] (MHz)
$P(6)$	...	1,741,122.646 (6895)
$P(4)$	...	1,787,890.569 (6895)
$P(2)$	...	1,836,821.195 (6895)
$Q(2)$	1,890,558.063	...
$Q(4)$	1,896,706.555	1,896,707.137 (899)
$Q(6)$	1,906,337.903	1,906,338.269 (899)
$R(0)$	1,914,274.133	...
$Q(8)$	1,919,410.760	...
$Q(10)$	1,935,870.177	...
$Q(12)$	1,955,648.963	...
$R(2)$	1,968,595.391	...
$Q(14)$	1,978,667.579	...
$Q(16)$	2,004,835.934	...
$R(4)$	...	2,025,051.586 (899)
$R(6)$	...	2,083,626.535 (899)

[a] Laser sideband measured line positions in units of cm^{-1} were converted to units of megahertz for easier comparison.

[b] Estimated systematic errors are ± 500 kHz.

3. THE LABORATORY SPECTRA OF THE BENDING VIBRATION OF C_3

The electronic ground state of C_3 is $X^1\Sigma$, and the ν_2 bending vibration displays a perpendicular spectrum with appropriately located P-, Q-, and R-branches, and the band origin has been determined by Schmuttenmaer et al. (1990) to be 63.416529(40) cm^{-1}. This center frequency, as refined from the recent Cologne measurements, is 1.9011821(8) THz.

Figure 2 shows two selected laboratory recordings of the $R(2)$ and $Q(12)$ transitions together with an overview of the entire calculated spectrum, displayed for reasons of clarity in stick format. This stick diagram is based on a fit of the recorded transitions measured in our Cologne and Berkeley laboratories. The parameters obtained from the fit agree within 2 σ error bars with the values published by the Berkeley group (Schmuttenmaer et al. 1990). The newly measured transition frequencies of the 10 lines reported in this Letter are summarized in Table 1 together with the seven transitions detected earlier by the Berkeley Group (Schmuttenmaer et al. 1990). Two transitions, i.e., $Q(4)$ and $Q(6)$, have been recorded in both laboratories and are found to agree within their determined line center positions and within their respectively quoted uncertainties. This excellent agreement between the Berkeley and Cologne data sets on C_3 and the additionally observed transitions furnish a

satisfying confirmation of the earlier assignment given by Schmuttenmaer et al. (1990).

The authors thank A. Betz and R. Boreiko for recording the data on board the KAO using the Betz/Boreiko receiver. The Berkeley group was supported by NASA Astrophysics and NASA Exobiology programs. R. J. S. thanks the Alexander von Humboldt Foundation for a Senior Scientist Award. The Cologne group has been supported by the Deutsche Forschungs-gemeinschaft via research grants SFB-301 and SFB-494. We kindly acknowledge the Ministry of Science of the Land Nordrhein-Westfalen/Germany for financial support.

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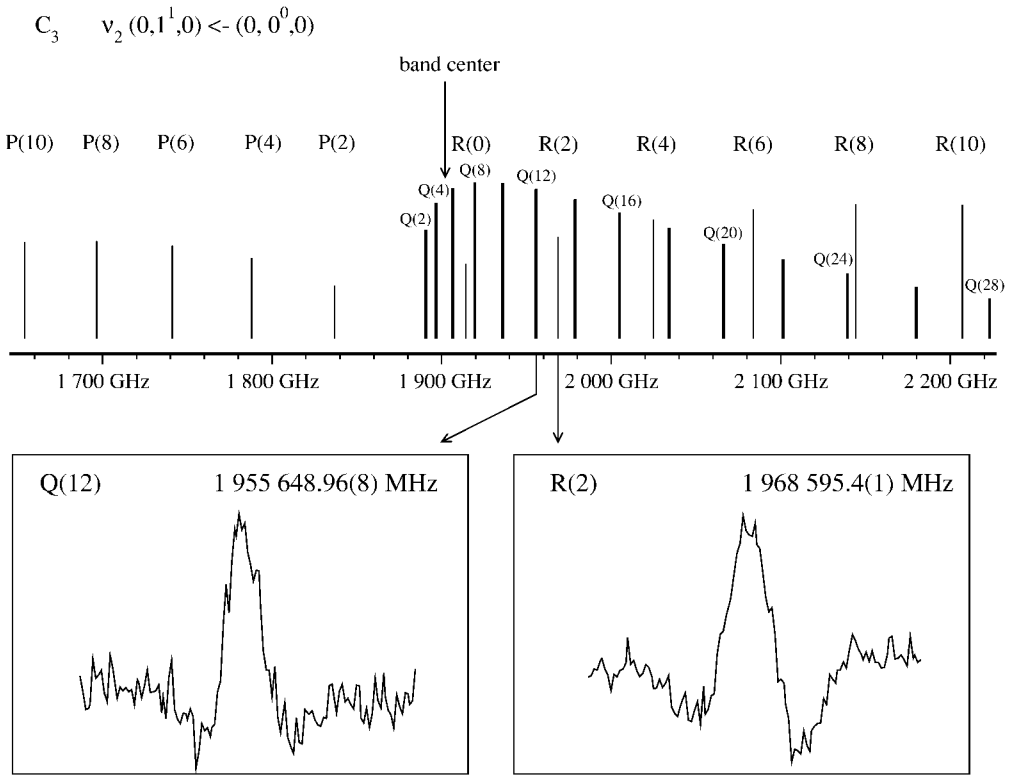
ERRATUM

In the Letter "Interstellar Detection of CCC and High-Precision Laboratory Measurements near 2 THz" by T. F. Giesen, A. O. Van Orden, J. D. Cruzan, R. A. Provencal, R. J. Saykally, R. Gendriesch, F. Lewen, and G. Winnewisser (ApJ, 551, L181 [2001]), there is an error in Figure 2. The *R*-branch transitions with $J = 4$, 6, 8, and 10 have been accidentally wrongly labeled as *R*(6), *R*(8), *R*(10), and *R*(12). They instead should read *R*(4), *R*(6), *R*(8), and *R*(10). The corrected Figure 2 is shown here.

In Table 1 the footnotes a and b are interchanged. Table 1 and the correct footnotes are shown here.



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